

Supplementary Material

Topological estimation of percolation thresholds

Richard A. Neher, Klaus Mecke and Herbert Wagner

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A combinatorial approach to the Euler Characteristic

In the main body of this paper, we introduced the Euler characteristic (EC) and calculated its mean value per site for percolation clusters on two dimensional lattices. The approach presented in the main text can be generalized to higher dimensional cell complexes where the EC is given by the alternating sum of the number of cells of different dimension.

Here, we want to present a complementary definition not restricted to cell complexes and better suited to study continuum percolation. Following the combinatorial approach (Hadwiger, 1955), we start with the family \mathcal{K}^d of closed, bounded, and convex subsets $A \subset \mathbb{R}^d$, $0 \leq \dim(A) \leq d$, and define the EC on \mathcal{K}^d by

$$\mathcal{X}(A) := \begin{cases} 1, & A \in \mathcal{K}^d \setminus \emptyset, \\ 0, & A = \emptyset \in \mathcal{K}^d. \end{cases} \quad (1)$$

Next, we construct a family \mathcal{R}^d of spatial patterns P by forming finite unions of convex bodies $A_i \in \mathcal{K}^d$, i.e. $P = \bigcup_{i=1}^n A_i$, and promote the EC to a valuation on the convex ring \mathcal{R}^d by requiring additivity (Hadwiger, 1955)

$$\mathcal{X}(A \cup B) := \mathcal{X}(A) + \mathcal{X}(B) - \mathcal{X}(A \cap B). \quad (2)$$

The value of $\mathcal{X}(A \cup B)$ is well-defined, since $A, B \in \mathcal{K}^d$ implies $A \cap B \in \mathcal{K}^d$. Iteration of Equation 2 leads to

$$\mathcal{X}\left(\bigcup_{i=1}^n A_i\right) = \sum_{k=1}^n (-1)^{k-1} \sum_{i_1 < i_2 < \dots < i_k} \mathcal{X}(A_{i_1} \cap A_{i_2} \dots \cap A_{i_k}), \quad (3)$$

for $A_1, \dots, A_n \in \mathcal{K}^d$. Hadwiger has shown that the combinatorial EC agrees with the Euler-Poincaré characteristic from algebraic topology, when the latter is restricted to the convex ring \mathcal{R}^d . It is now straightforward to turn these formal concepts into practical tools for the study of percolation clusters.

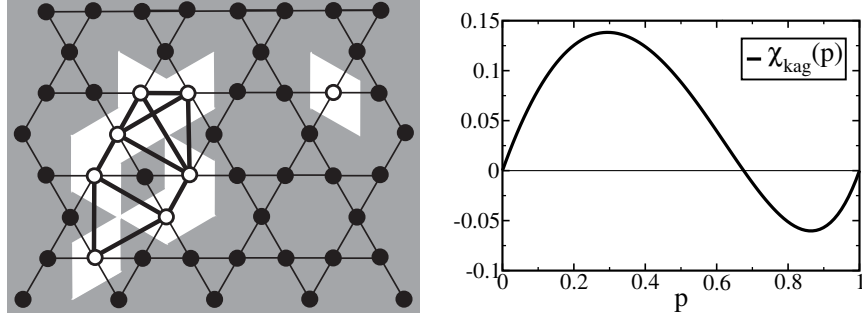


Figure 1: Clusters on the kagomé lattice. Left: To each white vertex, we attach a face of the dual lattice. White faces are connected if they share a dual edge or vertex, as indicated by the thick black lines. The white pattern displayed consists of two clusters \bar{P}_1 and \bar{P}_2 with $size(P_1) = 7$ and $size(P_2) = 1$. The EC of the pattern is given by $\mathcal{X}(\bar{P}_1 \cup \bar{P}_2) = \mathcal{X}(\bar{P}_1) + \mathcal{X}(\bar{P}_2) = 0 + 1$. Right: The MEC of white clusters for occupation probability \bar{p} .

At first, we want to reproduce the relations presented in the main text. To this end, consider site percolation on a finite planar 2-d lattice Λ with periodic boundary conditions and let each lattice vertex be white with probability \bar{p} and black with probability $p = 1 - \bar{p}$ ¹. To construct spatial patterns corresponding to the white vertices, we attach to each white vertex a face of the dual lattice Λ^* , as illustrated in Figure 1 for the kagomé lattice. The k -cells C_k^* of Λ^* , i.e. its vertices v^* , edges e^* and faces f^* for $k = 0, 1, 2$, are convex bodies as introduced previously and the EC of union of cells can be calculated using Equation 3. A white cluster is now defined as a maximal collection of white faces f^* with nonempty pairwise intersections. Since a face is closed, meaning its boundary ∂f^* is part of the face ($\partial f^* = f^* \cap \partial f^*$), two faces are connected if they share an edge e^* or only a vertex v^* . For example, the configuration of white cells on the kagomé lattice shown in Figure 1 forms a pattern of two clusters \bar{P}_1 and \bar{P}_2 .

In percolation theory, the occurrence of a pattern $\bar{P} = \cup_{i=1}^{n_2^*} f_i^* \in \mathcal{R}^2$ is a probabilistic event. Therefore, $\mathcal{X}(\bar{P})$ is now a random variable. Its mean value per site of the lattice Λ is defined by

$$\bar{\chi}(\bar{p}) = \lim_{N \rightarrow \infty} \frac{1}{N} \langle \mathcal{X} \left(\cup_{i=1}^{n_2^*} f_i^* \right) \rangle_{\bar{p}}, \quad (4)$$

where N is the number of vertices of Λ . To evaluate the average of the EC, we use the iterated additivity relation from Equation 3 with the A_i replaced by f_i^* , $i = 1, \dots, n_2^*$. The task is simplified by writing a *closed* polyhedral face f^* as the union of its *disjoint* open components (open interior \check{f}^* together with the

¹Within the combinatorial approach, the connectivities of white vertices are more natural than the connectivities of black vertices; we therefore start out with a white pattern and recover the black patterns by complementation later.

open edges \check{e}^* and the vertices \check{v}^* from the boundary ∂f^*), and adopting the definition (Nef, 1981; Likos et al., 1995)

$$\mathcal{X}(\check{C}_k^*) = (-1)^k, \quad k = 0, 1, 2, \quad (5)$$

for the EC of open k -dimensional lattice cells. With this representation of a white pattern, we obtain

$$\begin{aligned} \mathcal{X}\left(\cup_{i=1}^{n_2^*} f_i^*\right) &= \sum_{i=1}^{n_2^*} \mathcal{X}(\check{f}_i^*) + \sum_{i=1}^{n_1^*} \mathcal{X}(\check{e}_i^*) + \sum_{i=1}^{n_0^*} \mathcal{X}(\check{v}_i^*) \\ &= n_2^* - n_1^* + n_0^* = n_0 - n_1 + n_2. \end{aligned} \quad (6)$$

Here n_k^* , $k = 0, 1, 2$ denotes the number of white faces, edges and vertices of the pattern on Λ^* and the last equality follows from duality. The average of the EC depends on the specific geometry of the underlying lattice. As an example, let us consider the eleven Archimedean lattices (comp. main text, (Grünbaum and Shephard, 1986)). In an Archimedean lattice with vertex type (n_1, \dots, n_z) and periodic boundary conditions, the fractional numbers of bonds and polygonal faces with n_i edges per site of the lattice Λ are given by $\frac{z}{2}$ and $\frac{1}{n_i}$, respectively. With this structural information, we find the averages

$$\begin{aligned} \frac{1}{N} \langle n_2^* \rangle &= \bar{p}, \\ \frac{1}{N} \langle n_1^* \rangle &= \frac{z}{2} (1 - p^2), \\ \frac{1}{N} \langle n_0^* \rangle &= \sum_{i=1}^z \frac{1}{n_i} (1 - p^{n_i}). \end{aligned} \quad (7)$$

These expressions are obtained by noting that a face f_i^* is white with probability $\bar{p} = 1 - p$; an edge e_i^* is white with probability $1 - p^2$, since it belongs to a white pattern if at least one of the faces sharing e_i^* is white; likewise, a vertex v_i^* is white, if at least one of the faces sharing v_i^* is white, and this happens with probability $1 - p^{n_i}$. Thus from Eq. 5, 6 and 7, we arrive at the result

$$\bar{\chi}(\bar{p}) = p - [1 - (1 - \bar{p})^2] \frac{z}{2} + \sum_i \frac{a_i}{n_i} [1 - (1 - \bar{p})^{n_i}] \quad (8)$$

for the MEC of percolation patterns on Archimedean lattices. For example, Equation 8 yields for the kagomé lattice (3, 6, 3, 6)

$$\bar{\chi}_{kag}(\bar{p}) = \bar{p}(1 - \bar{p}) \left(1 - 4\bar{p} + \frac{10}{3}\bar{p}^2 - \frac{5}{3}\bar{p}^3 + \frac{1}{2}\bar{p}^4 \right), \quad (9)$$

and for the triangular lattice

$$\bar{\chi}_{tri}(\bar{p}) = \bar{p}(1 - \bar{p}) (1 - 2\bar{p}). \quad (10)$$

A given white pattern $\bar{P} = \cup_{j=1}^{n_2^*} f_j^*$ determines a unique black pattern P , as the set-complement, \bar{P}_{comp} , of \bar{P} with respect to the lattice Λ , and we have

$$\mathcal{X}(P \cup \bar{P}) = \mathcal{X}(P) + \mathcal{X}(\bar{P}) = 0. \quad (11)$$

The first equality holds because $P \cap \bar{P} = \emptyset$ by definition of the complement, the second equality follows since $P \cup \bar{P}$ is topologically a two dimensional torus.

Obviously, the complementary pattern P may be viewed as an aggregate of percolation clusters of faces of Λ^* chosen with probability $p = 1 - \bar{p}$ and colored black. The MEC of black patterns is defined by

$$\chi(p) = \lim_{N \rightarrow \infty} \frac{1}{N} \langle \mathcal{X}(P) \rangle_p. \quad (12)$$

Consequently, Equation 11 implies the symmetry-type relation

$$\bar{\chi}(1 - p) + \chi(p) = 0. \quad (13)$$

Thus, the MEC of black patterns is obtained from that of white patterns via simple substitution. After substitution, we obtain exactly the same polynomials for $\chi(p)$ as in the main text, for example:

$$\begin{aligned} \chi_{kag}(p) &= p(1 - p) \left(1 - p - \frac{1}{3}(p^2 + p^3 + p^4) \right), \\ \chi_{tri}(p) &= p(1 - p)(1 - 2p) = \bar{\chi}_{tri}(p) \end{aligned} \quad (14)$$

We note, that the triangular lattice is the only one among the Archimedian lattice with equal “black” and “white” MECs.

Summary of two-dimensional lattices

In this section, we collect all formulae for the mean Euler characteristic of the various lattices discussed in the main text and present tables containing the numerical values of p_0 , p^* , and p_c . We also discuss some irregular lattices and the dual Archimedean lattices, which are not included in the main paper. MapleTM sheets used to calculate the MECs as well as numerical values of p_0 and p^* are available from the authors on request.

Archimedean lattices – site percolation

Each vertex of an Archimedean lattice is surrounded by z regular polygons with n_1, \dots, n_z edges. In terms of the n_i , the MEC of an Archimedean lattice is given by

$$\chi(p) = p(1-p) \left(1 - p \sum_{i=1}^z \frac{1}{n_i} \sum_{\mu=0}^{n_i-3} p^\mu \right). \quad (15)$$

The vertex configurations, and a comparison of the zero crossing, our estimator of p_c , and the actual threshold are given in Table 1.

n_1, \dots, n_z	p_0	p^*	p_c^{site}
3, 12, 12	0.8395	0.7869	0.807900...
4, 6, 12	0.7833	0.7373	0.747806(4)
4, 8, 8	0.7689	0.7269	0.729724(3)
6, 6, 6	0.7413	0.7043	0.697043(3)
3, 6, 3, 6	0.6756	0.6462	0.6527036...
3, 4, 6, 4	0.6468	0.6224	0.621819(3)
4, 4, 4, 4	0.6180	0.5987	0.5927460(5)
3, 3, 3, 3, 6	0.5913	0.5752	0.579498(3)
3, 3, 4, 3, 4	0.5616	0.5511	0.550806(3)
3, 3, 3, 4, 4	0.5616	0.5511	0.550213(3)
3, 3, 3, 3, 3, 3	0.5	0.5	0.5

Table 1: Archimedean lattices – site percolation. Lattices are ordered with decreasing p_c , the percolation thresholds are from Suding and Ziff (1999) and references therein. These values are plotted in Figure 3 of the main paper.

Archimedean lattices – bond percolation

The MEC of the covering lattice of an Archimedean lattice with vertex type n_1, \dots, n_z is given by

$$\chi(p) = -p + \frac{2}{z} (1 - (1-p)^z) + \sum_i \frac{2}{zn_i} p^{n_i}. \quad (16)$$

n_1, \dots, n_z	p_0	p^*	p_c^{bond}
3, 12, 12	0.7580	0.7098	0.7404219(8)
4, 6, 12	0.7054	0.6685	0.6937338(7)
4, 8, 8	0.6964	0.6623	0.6768023(6)
6, 6, 6	0.6756	0.6462	0.6527036...
3, 6, 3, 6	0.5277	0.5227	0.5244053(3)
3, 4, 6, 4	0.5134	0.5111	0.5248325(5)
4, 4, 4, 4	0.5	0.5	0.5
3, 3, 3, 3, 6	0.4069	0.4233	0.4343062(5)
3, 3, 4, 3, 4	0.3992	0.4166	0.4141374(5)
3, 3, 3, 4, 4	0.3992	0.4166	0.4196419(4)
3, 3, 3, 3, 3, 3	0.3244	0.3538	0.3472963...

Table 2: Archimedean lattices – bond percolation. Lattices are in the same order as in Table 1, numerical estimates of percolation thresholds are from Parviainen (2007). This data is plotted in Figure 3 of the main paper.

Dual Archimedean lattices – site percolation

The MEC of the dual lattice of an Archimedean lattice depends only on the coordination number of the Archimedean lattice.

$$\chi(p) = p(1-p) \left(1 - \frac{2}{z-2} \sum_{i=1}^{z-2} p^i \right) \quad (17)$$

A graph illustrating the relationship between p_c and the zero crossing of the MEC and the performance of our estimator p^* is shown in Figure 2. The dual Archimedean lattices are also known as Laves lattices.

dual(n_1, \dots, n_z)	p_0	p^*	p_c^{site}
dual(3, 12, 12)	0.5	0.5	0.5
dual(4, 6, 12)	0.5	0.5	0.5
dual(4, 8, 8)	0.5	0.5	0.5
dual(6, 6, 6)	0.5	0.5	0.5
dual(3, 6, 3, 6)	0.6180	0.5987	0.5848(2)
dual(3, 4, 6, 4)	0.6180	0.5987	0.5824(2)
dual(4, 4, 4, 4)	0.6180	0.5987	0.5927460(5)
dual(3, 3, 3, 3, 6)	0.6914	0.6612	0.6396(2)
dual(3, 3, 4, 3, 4)	0.6914	0.6612	0.6500(2)
dual(3, 3, 3, 4, 4)	0.6914	0.6612	0.6476(2)
dual(3, 3, 3, 3, 3, 3)	0.7413	0.7043	0.697043(3)

Table 3: Dual Archimedean lattices – site percolation. Lattices are in the same order as in Table 1, numerical estimates of percolation thresholds are from (van der Marck, 2003); see Figure 2 for a plot of this data.

2-uniform lattices – site percolation

While Archimedean lattice have only one vertex type, the vertices of 2-uniform lattices are of two distinct types. A vertex is again characterized by the polygons surrounding it. Each vertex type i makes up a fraction s_i of the total vertices and a 2-uniform lattice is typically denoted by $s_1(n_1^1, \dots, n_{z_1}^1) + s_2(n_1^2, \dots, n_{z_2}^2)$. The MEC can be expressed in terms of the vertex configuration:

$$\chi(p) = p(1-p) \left(1 - p \sum_{\nu=1,2} \sum_{i=1}^{z_\nu} \frac{s_\nu}{n_i^\nu} \sum_{\mu=0}^{n_i^\nu-3} p^\mu \right). \quad (18)$$

We determined the percolation thresholds of all 2-uniform lattices using the algorithm by Newman and Ziff (Newman and Ziff, 2001). Simulation were performed on lattices with linear dimension $L = 64, 128, 256, 512$ and 1024 . The probabilities at which a spanning appears on a finite lattice were extrapolated to infinite lattice size using the well known finite size scaling relations.

$s_1(n_1^1, \dots, n_{z_1}^1) + s_2(n_1^2, \dots, n_{z_2}^2)$	p_0	p^*	p_c^{site}
$\frac{1}{2}(3, 4, 3, 12) + \frac{1}{2}(3, 12^2)$	0.7909	0.7403	0.7680(2)
$\frac{1}{3}(3, 4, 6, 4) + \frac{2}{3}(4, 6, 12)$	0.7424	0.7016	0.7157(2)
$\frac{1}{5}(3^6) + \frac{6}{7}(3^2, 4, 12)$	0.6918	0.6555	0.6808(2)
$\frac{2}{7}(3^2, 6^2) + \frac{1}{3}(3, 6, 3, 6)$	0.6756	0.6462	0.6499(2)
$\frac{1}{7}(3^6) + \frac{6}{7}(3^2, 6)$	0.6532	0.6270	0.6329(2)
$\frac{1}{4}(3, 4^2, 6) + \frac{1}{5}(3, 6, 3, 6)$	0.6526	0.6271	0.6286(2)
$\frac{1}{4}(3, 4^2, 6) + \frac{1}{5}(3, 6, 3, 6)$	0.6526	0.6271	0.6279(2)
$\frac{1}{3}(3, 4^2, 6) + \frac{1}{3}(3, 4, 6, 4)$	0.6468	0.6224	0.6221(2)
$\frac{1}{2}(3^4, 6) + \frac{1}{2}(3^2, 6^2)$	0.6354	0.6119	0.6171(2)
$\frac{1}{2}(3^3, 4^2) + \frac{1}{2}(3, 4, 6, 4)$	0.6053	0.5874	0.5885(2)
$\frac{1}{2}(3^2, 4, 3, 4) + \frac{1}{2}(3, 4, 6, 4)$	0.6053	0.5874	0.5883(2)
$\frac{1}{2}(3^3, 4^2) + \frac{1}{2}(4^4)$	0.5907	0.5755	0.5720(2)
$\frac{2}{3}(3^3, 4^2) + \frac{1}{3}(4^4)$	0.5811	0.5675	0.5648(2)
$\frac{1}{4}(3^6) + \frac{3}{2}(3^4, 6)$	0.5684	0.5563	0.5607(2)
$\frac{1}{2}(3^3, 4^2) + \frac{1}{2}(3^2, 4, 3, 4)$	0.5616	0.5511	0.5505(2)
$\frac{1}{3}(3^3, 4^2) + \frac{2}{3}(3^2, 4, 3, 4)$	0.5616	0.5511	0.5504(2)
$\frac{1}{4}(3^6) + \frac{6}{7}(3^2, 4, 3, 4)$	0.5530	0.5439	0.5440(2)
$\frac{1}{2}(3^6) + \frac{1}{2}(3^4, 6)$	0.5453	0.5374	0.5407(2)
$\frac{1}{3}(3^6) + \frac{2}{3}(3^3, 4^2)$	0.5414	0.5343	0.5342(2)
$\frac{1}{2}(3^6) + \frac{1}{2}(3^3, 4^2)$	0.5311	0.5258	0.5258(2)

Table 4: 2-uniform lattices – site percolation. Lattices are ordered according to decreasing percolation threshold. Compare with Figure 3 of the main paper.

Irregular lattices

For lattices that are not included in any of the above classes, we present the polynomials $\chi(p)$ here. Table 5 and Figure 3 summarize our results for

site percolation: Laves lattices

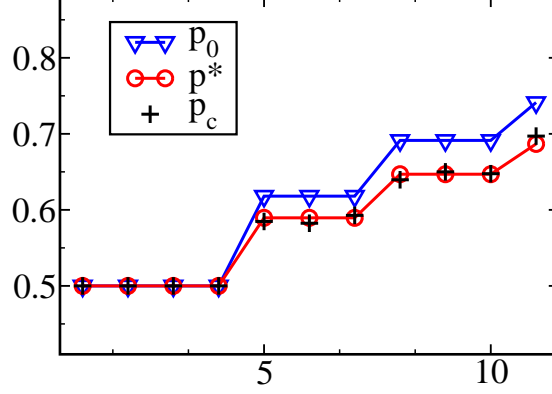


Figure 2: Dual Archimedean lattices – site percolation. The solution of Equation 18 of the main text, p^* , is a good estimate of p_c^{site} for all dual Archimedean lattices, also known as Laves lattices. For numerical values of p_0 , p^* and p_c , see Table 3.

irregular lattices.

In addition to the Archimedean lattices, a number of other lattices have been studied by Suding and Ziff (1999), including the *bowtie* lattice with vertex configuration $\frac{1}{2}(3^4, 4^2) + \frac{1}{2}(3^2, 4^2)$ the *dual bowtie* lattice with vertex configuration $\frac{1}{3}(4^2, 6^2) + \frac{2}{3}(4, 6^2)$. Given these vertex configurations, $\chi(p)$ can be calculated using the same formula as for 2-uniform lattices.

Voronoi tessellation and its dual. Consider points randomly and independently distributed on the plane and construct faces around these points using the Wigner-Seitz construction. The resulting Voronoi tessellation of the plane consists of faces each of which contains exactly one of the randomly distributed points. The faces have six sides on average and the coordination number of a vertex is three with probability one. The dual of the Voronoi tessellation is a completely triangulated lattice with the randomly distributed points as vertices. The MEC of the dual tessellation is therefore the same as that of the triangular lattice. To calculate the MEC of the Voronoi lattice, we need to know the distribution ν_i of the faces with different number of sides. This is known approximately (D. Stoyan, 1996) and the MEC is found to be

$$\chi_{vor}(p) = p - 1 + \frac{3}{2}(1 - p^2) - \frac{1}{2} \sum_{i \geq 3} \nu_i (1 - p^i). \quad (19)$$

We are not aware of any estimation of the site percolation threshold for the Voronoi tessellation.

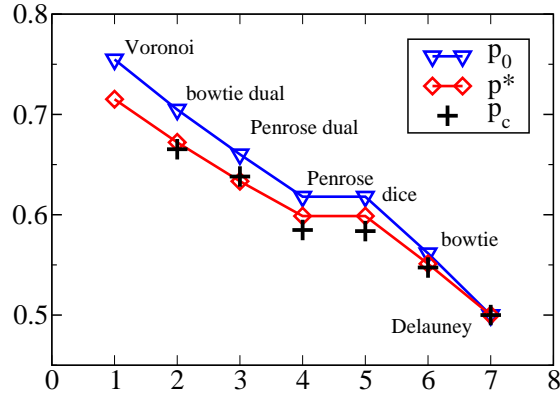


Figure 3: Irregular lattices – site percolation. The relationship between p_0 , p^* and p_c^{site} also holds for irregular, random and quasi-periodic lattices. For numerical values, see Table 5.

lattice	$s_1(n_1^1, \dots, n_{z_1}^1) + s_2(n_1^2, \dots, n_{z_2}^2)$	p_0	p^*	p_c^{site}
bowtie	$\frac{1}{2}(3, 3, 3, 3, 4, 4) + \frac{1}{2}(3, 3, 4, 4)$	0.5616	0.5511	0.5474(8)
bowtie dual	$\frac{1}{3}(4, 4, 6, 6) + \frac{2}{3}(4, 6, 6)$	0.7048	0.6722	0.6649(3)
dice	$\frac{1}{3}(4, 4, 4, 4, 4, 4) + \frac{2}{3}(4, 4, 4)$	0.6180	0.5987	0.5848(2)
Penrose		0.6180	0.5987	0.5837(2)
Penrose dual		0.6602	0.6334	0.6381(3)
Voronoi		0.7548	0.7151	–
Voronoi dual		0.5	0.5	0.5

Table 5: Irregular lattices – site percolation. Percolation thresholds are taken from (van der Marck, 1997; Yonezawa et al., 1988). This data is plotted in Figure 3.

Penrose tiling and its dual. The rhombic Penrose tiling is a quasi periodic lattice consisting of 4-sided polygons only. The vertices have an average coordination number of 4, varying between 3 and 7. The distribution of the different vertex types is known (Lu and Birman, 1987), but since the tessellation consists of 4-sided polygons only, the MEC is the same as that of the square lattice. The dual Penrose tiling, however, has faces with 3 to 7 sides. The coordination number is uniformly $z = 4$, and from the distribution of faces we find for the MEC

$$\chi(p) = -(1-p) + 2(1-p^2) - \sum_{i \geq 3} \nu_i (1-p^i), \quad (20)$$

where ν_i is the probability that a given face has i sides (Lu and Birman, 1987). The percolation thresholds, p_0 and p^* for these lattices are given in Table 5.

Three dimensional cubic lattices

The generalization of Equation 5 to three dimensions states that the MEC of the white pattern is given by the alternating sum of the mean number of cells of different dimensions per vertex. For cubic lattices, natural space filling cells are given by the Wigner-Seitz cells. While white vertices are connected whenever their cells share a face, an edge or a vertex, black vertices are connected only when their cells share a face. For the simple cubic lattice, the MEC is given by

$$\chi_{sc}(p) = p - 3p^2 + 3p^4 - p^8. \quad (21)$$

The MEC of the face centered cubic (fcc) lattice is given by

$$\chi^{fcc}(p) = p(1-p)(p^4 + p^3 + 3p^2 - 5p + 1). \quad (22)$$

A vertex of the fcc-lattice has 12 nearest neighbors, each of which corresponds to one face of the WSC.

A vertex of the bcc-lattice is connected to eight neighbors. The Wigner-Seitz cell, however, has 14 faces, six of which make contact to next nearest neighbors on the lattice. The MEC obtained when using the connectivities of the Wigner-Seitz cells corresponds to a lattice where the six next nearest neighbors are adjacent.

$$\chi_{14-14}^{bcc}(p) = p(1-p)(6p^2 - 6p + 1) \quad (23)$$

The MEC of the bcc-lattice for black and white vertices are identical, reflecting the fact that at any 1-cell (edge) or a 0-cell (vertex) of the WSC no cells meet that do not share a face.

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